

US EPA ARCHIVE DOCUMENT

TABLE A-3-151

## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	139.11
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	386.1
$V_p$ (atm)	$V_p$ value cited in Howard (1989-1993).	--	1.32E-06 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Howard (1989-1993).	--	2.50E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.32E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.30E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.61E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.13E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.37E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.37E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.28E+01

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## CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.75E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	2.09E+02
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.32E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.01E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.05E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.05E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	8.26E+02

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CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	8.26E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.46E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.04E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.47E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.46E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.61E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.67E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	6.20E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.17E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

## TABLE A-3-151

### CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-152

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	$MW$ value cited in U.S. EPA (1995b)	--	158.20
$T_m$ (K)	--	--	NA
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	3.80E-04 at 25°C
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	1.10E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.47E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.50E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	7.52E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	2.57E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.07E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.07E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.05E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.29E+00

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## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
$F_v$ (unitless)	$F_v$ value cited in NC DEHNR (1997).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.30E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.14E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.57E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.57E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.77E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.77E-01

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## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.04E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.46E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.82E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.04E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.10E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.00E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	5.4E+00
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.6E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	5.4E+00

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	198.23
$T_m$ (K)	Montgomery and Welkom (1991)	--	339.6
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.74E-07 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	3.50E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.84E-07
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.12E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.35E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.06E+03
$K_{oc}$ (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	--	3.27E+02, for pH range of 4.9 to 8.0
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.27E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.45E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.31E+01

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## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.61E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.71E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.89E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.89E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.51E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.51E+01

TABLE A-3-153

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.45E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.67E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.24E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.45E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.11E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.18E+02
$BAF_{fish}$ (L/kg, FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997b)	C-1-7	4.9E-03
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	1.4E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	4.9E-03

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-154

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	130.19
$T_m$ (K)	--	--	ND
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1992a).	--	6.09E-06 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1992a).	--	1.46E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.43E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.67E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.75E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b).	--	2.40E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.70E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.70E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.28E+00

TABLE A-3-154

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.80E-01
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.99E+00
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.29E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.17E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.17E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.04E+01

TABLE A-3-154

## CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (continued)</b>			
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.04E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.91E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.03E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.30E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.91E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.76E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.59E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)		C-1-8	ND
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	7.0E+00
$RfC$ (mg/m <sup>3</sup> )		C-2-3	ND
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	2.0E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-2-2	7.0E+00

Note:

NA = Not applicable

## TABLE A-3-154

### CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-155

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	460.76
$T_m$ (K)	U.S. EPA (1994a)	--	598.1
$V_p$ (atm)	U.S. EPA (1994a)	--	8.61E-11 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	4.00E-07
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.00E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.06E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.69E-07
$K_{ow}$ (unitless)	U.S. EPA (1994a)	--	3.89E+07
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.40E+07
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.40E+05
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.80E+06



TABLE A-3-155

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)**

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.60E+05
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	9.93E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.62E+05
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	6.77E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.59E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.59E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.60E+06

TABLE A-3-155

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)**

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.60E+06
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
<b>Biotransfer Factors for Animals (Continued)</b>			
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	9.90E-03
$Ba_{chicken}$ (unitless, FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.10E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.001
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-155**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-156

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	444.76
$T_m$ (K)	U.S. EPA (1994a)	--	531.1
$V_p$ (atm)	U.S. EPA (1994a)	--	4.93E-15 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	1.20E-06
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.90E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.48E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.78E-06
$K_{ow}$ (unitless)	U.S. EPA (1994a)	--	6.03E+08
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.72E+08
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.72E+06
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.79E+07

TABLE A-3-156

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)**

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.49E+07
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.10E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.67E-03
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.34E+06
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.60E-01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.26E-04
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.26E-04
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.30E+06

TABLE A-3-156

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.30E+06
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	7.92E-03
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (see Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	4.40E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.001
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-156**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-157

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	356.42
$T_m$ (K)	U.S. EPA (1994a)	--	513.1
$V_p$ (atm)	U.S. EPA (1994a)	--	1.25E-12 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.20E-04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.60E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.21E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.38E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	4.37E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.69E+06
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05



TABLE A-3-157

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.08E+05
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.19E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.12E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.62E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.62E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.20E+05

**TABLE A-3-157**  
**CHEMICAL-SPECIFIC INPUTS FOR**  
**1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.20E+05
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.71E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.50E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.50
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

Note:

**TABLE A-3-157**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)**

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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**TABLE A-3-158**

**CHEMICAL-SPECIFIC INPUTS FOR**  
**1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	340.42
$T_m$ (K)	U.S. EPA (1994a)	--	498.1
$V_p$ (atm)	U.S. EPA (1994a)	--	3.58E-12 at 25°C (solid)
$S$ (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	2.40E-04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	6.17E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.80E+06
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+05

TABLE A-3-158

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.52E+05
$ksg$ (year) <sup>-1</sup>	$ksg$ value assumed to be the same as the $ksg$ value calculated for 2,3,4,7,8-PentaCDF. $ksg$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
$Fv$ (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that are provided in this table. $Vp$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	3.64E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.93E+04
$Br_{rootveg}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.03E+00
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.61E-03
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.61E-03
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04

**TABLE A-3-158**

**CHEMICAL-SPECIFIC INPUTS FOR**

**1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	2.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.09E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.31E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	ND
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.05
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-158**

**CHEMICAL-SPECIFIC INPUTS FOR  
1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)**

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Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

**TABLE A-3-159**  
**CHEMICAL-SPECIFIC INPUTS FOR**  
**2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	340.42
$T_m$ (K)	U.S. EPA (1994a)	--	469.1
$V_p$ (atm)	U.S. EPA (1994a)	--	4.33E-12 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	2.36E-04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated by using Equation A-3-2. Recommended value was calculated by using the $MW$ and $D_a$ values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	8.32E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.13E+06
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+05



TABLE A-3-159

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.05E+05
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.63E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.95E+04
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	9.65E-01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.87E-03
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.87E-03
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04

**TABLE A-3-159**

**CHEMICAL-SPECIFIC INPUTS FOR**

**2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	9.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	4.89E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	5.91E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.32E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.50
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-159**

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-160

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	250.34
$T_m$ (K)	Montgomery and Welkom (1991)	--	358.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994f)	--	3.10E-06 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	--	3.20E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.86E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.34E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.22E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.21E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.21E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.41E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.29E+03

TABLE A-3-160

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.33E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.93E+03
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	5.99E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.44E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.44E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.04E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.04E-01

TABLE A-3-160

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.72E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.07E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.72E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.72E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.43E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.61E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.8E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-161

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	295.36
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	417.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993)	--	3.1E-06 at 25°C (solid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	--	3.20E-02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.86E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	5.0E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	4.37E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.89E+03
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02



TABLE A-3-161

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.36E+02
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.62E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.49E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.06E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.06E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.71E-01



TABLE A-3-161

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.71E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.47E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.10E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.33E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	8.66E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.65E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.03E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	2.6E-01
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	7.4E-05
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.6E-01

## TABLE A-3-161

### CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-162

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	266.35																														
$T_m$ (K)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	463																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.11E-07 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.34E+01																														
$H$ (atm·m³/mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.41E-05																														
$D_a$ (cm²/s)	$D_a$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.56E-02																														
$D_w$ (cm²/s)	$D_w$ value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	8.01E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.20E+05																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>19,949</td></tr><tr><td>2</td><td>19,918</td></tr><tr><td>3</td><td>19,604</td></tr><tr><td>4</td><td>16,942</td></tr><tr><td>5</td><td>7,333</td></tr><tr><td>6</td><td>1,417</td></tr><tr><td>7</td><td>504.9</td></tr><tr><td>8</td><td>408.7</td></tr><tr><td>9</td><td>399.1</td></tr><tr><td>10</td><td>398.1</td></tr><tr><td>11</td><td>398.0</td></tr><tr><td>12</td><td>398.0</td></tr><tr><td>13</td><td>398.0</td></tr><tr><td>14</td><td>398.0</td></tr></table>	pH	$K_{oc}$	1	19,949	2	19,918	3	19,604	4	16,942	5	7,333	6	1,417	7	504.9	8	408.7	9	399.1	10	398.1	11	398.0	12	398.0	13	398.0	14	398.0
pH	$K_{oc}$																																
1	19,949																																
2	19,918																																
3	19,604																																
4	16,942																																
5	7,333																																
6	1,417																																
7	504.9																																
8	408.7																																
9	399.1																																
10	398.1																																
11	398.0																																
12	398.0																																
13	398.0																																
14	398.0																																
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>199.5</td></tr><tr><td>2</td><td>199.2</td></tr><tr><td>3</td><td>196.0</td></tr><tr><td>4</td><td>169.4</td></tr><tr><td>5</td><td>73.33</td></tr><tr><td>6</td><td>14.17</td></tr><tr><td>7</td><td>5.05</td></tr><tr><td>8</td><td>4.09</td></tr><tr><td>9</td><td>3.99</td></tr><tr><td>10</td><td>3.98</td></tr><tr><td>11</td><td>3.98</td></tr><tr><td>12</td><td>3.98</td></tr><tr><td>13</td><td>3.98</td></tr><tr><td>14</td><td>3.98</td></tr></table>	pH	$K_{oc}$	1	199.5	2	199.2	3	196.0	4	169.4	5	73.33	6	14.17	7	5.05	8	4.09	9	3.99	10	3.98	11	3.98	12	3.98	13	3.98	14	3.98
pH	$K_{oc}$																																
1	199.5																																
2	199.2																																
3	196.0																																
4	169.4																																
5	73.33																																
6	14.17																																
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9	3.99																																
10	3.98																																
11	3.98																																
12	3.98																																
13	3.98																																
14	3.98																																

TABLE A-3-162

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	<p>pH <math>K_{oc}</math></p> <p>1 1,496</p> <p>2 1,494</p> <p>3 1,470</p> <p>4 1,271</p> <p>5 550.0</p> <p>6 106.2</p> <p>7 37.87</p> <p>8 30.66</p> <p>9 29.93</p> <p>10 29.86</p> <p>11 29.85</p> <p>12 29.85</p> <p>13 29.85</p> <p>14 29.85</p>
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	<p>pH <math>K_{oc}</math></p> <p>1 798.0</p> <p>2 796.7</p> <p>3 784.1</p> <p>4 677.7</p> <p>5 293.3</p> <p>6 56.67</p> <p>7 20.20</p> <p>8 16.35</p> <p>9 15.96</p> <p>10 15.92</p> <p>11 15.92</p> <p>12 15.92</p> <p>13 15.92</p> <p>14 15.92</p>
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.42E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.90E+03
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.77E+02

TABLE A-3-162

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
$Br_{ag}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}}\right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.48E-02
$Br_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}}\right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.48E-02
$Bv_{ag}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature(T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.02E+03
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.02E+03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.55E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.02E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.66E-03
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.55E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.39E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.97E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			

TABLE A-3-162

## CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
<i>RfD</i> (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.0E-02
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	1.2E-01
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-01
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from <i>Oral CSF</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	3.4E-05
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	Value based on the Oral CSF assuming route-to-route extrapolation	C-2-2	1.2E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-163

## CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.22
$T_m$ (K)	Montgomery and Welkom (1991)	--	371.1
$V_p$ (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	--	1.35E-03 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in Lucius et al. (1992).	--	1.28E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.88E-01
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.33E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.47E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.55E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.01E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.01E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.76E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.01E+03



TABLE A-3-163

## CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.26E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.47E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.49E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	9.08E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	9.08E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.08E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.08E-02

TABLE A-3-163

## CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.82E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.92E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.08E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.82E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.04E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	Default $BAF$ value recommended for use by U.S. EPA (1995b), when literature data were not available.	B-4-27	3.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-164

## CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	94.11																														
$T_m$ (K)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	314.0																														
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	5.74E-04 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	9.08E+04																														
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.95E-07																														
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.27E-02																														
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.00E+01																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>22.0</td></tr><tr><td>2</td><td>22.0</td></tr><tr><td>3</td><td>22.0</td></tr><tr><td>4</td><td>22.0</td></tr><tr><td>5</td><td>22.0</td></tr><tr><td>6</td><td>22.0</td></tr><tr><td>7</td><td>22.0</td></tr><tr><td>8</td><td>21.8</td></tr><tr><td>9</td><td>20.0</td></tr><tr><td>10</td><td>11.2</td></tr><tr><td>11</td><td>2.27</td></tr><tr><td>12</td><td>0.51</td></tr><tr><td>13</td><td>0.32</td></tr><tr><td>14</td><td>0.30</td></tr></table>	pH	$K_{oc}$	1	22.0	2	22.0	3	22.0	4	22.0	5	22.0	6	22.0	7	22.0	8	21.8	9	20.0	10	11.2	11	2.27	12	0.51	13	0.32	14	0.30
pH	$K_{oc}$																																
1	22.0																																
2	22.0																																
3	22.0																																
4	22.0																																
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10	11.2																																
11	2.27																																
12	0.51																																
13	0.32																																
14	0.30																																
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.20E-01																														

TABLE A-3-164

## CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.65E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.79E-01
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E+01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.50E+00
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-9; B-2-10; B-3-9	4.32E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.42E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-10	5.42E+00

TABLE A-3-164

## CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-9	3.52E+00
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	3.52E+00
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.38E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.54E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.12E-07
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.38E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.95E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	7.81E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-164

## CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks</b>			
<i>RfD</i> (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-01
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.1E+00
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-165

## CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	260.4
$T_m$ (K)	--	--	ND
$V_p$ (atm)	$V_p$ value cited in Montgomery and Welkom (1991).	--	1.70E-06 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	3.80E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.16E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.05E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.88E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.33E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.33E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.96E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.31E+01



TABLE A-3-165

## CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.06E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.55E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.43E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.43E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.48E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.48E+01



TABLE A-3-165

## CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.13E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.62E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.96E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.13E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.28E-04
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.63E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997c)	C-1-8	2.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E-04
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-166

## CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	148.11
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	403.9
$V_p$ (atm)	Howard (1989-1993)	--	2.63E-07 at 25°C (solid)
$S$ (mg/L)	Howard (1989-1993)	--	6.20E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.28E-09
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.04E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.97E-06
$K_{ow}$ (unitless)	NC DEHNR (1997)	--	2.5E-01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.80E-01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.80E-03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.60E-02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.92E-02

TABLE A-3-166

## CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.35E+04
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.39E+00
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.33E+03
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.63E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.63E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.03E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.03E+00

TABLE A-3-166

## CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.99E-09
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.28E-09
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	7.60E-09
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.99E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.96E-09
$BCF_{fish}$ (L/kg, FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.05E-01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.0E+00
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	1.2E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-167

## CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	256.13
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	428.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	5.30E-07 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	1.50E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.05E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.71E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.45E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	3.24E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	7.74E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.74E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.81E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.10E+01

TABLE A-3-167

## CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.23E+02
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.59E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	3.62E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	3.62E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.38E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.38E+01

TABLE A-3-167

## CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.57E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.13E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	9.84E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.57E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.42E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.74E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.5E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.6E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-168

## CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	202.24
$T_m$ (K)	Montgomery and Welkom (1991)	--	429.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	7.36E-12 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	1.30E-01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.14E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.72E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.14E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+05
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.80E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.80E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.10E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.72E+03



TABLE A-3-168

## CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992)	B-1-2; B-2-2; B-3-2; B-4-2	1.33E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.196
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.66E+03
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.44E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.98E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.98E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.04E+06
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.04E+06

**TABLE A-3-168**  
**CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.98E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.52E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.06E-03
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.98E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.99E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.19E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-169

## CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	79.10
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	231.5
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	2.60E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	3.00E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.86E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.10E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.08E-05
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.68E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.72E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.72E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.54E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.89E-01

TABLE A-3-169

## CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.07E+00
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.50E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.59E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.59E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.22E-05
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.22E-05

TABLE A-3-169

## CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.72E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.18E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.42E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.72E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.28E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.90E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.50E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-170

## CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	321.57
$T_m$ (K)	Montgomery and Welkom (1991)	--	314.1
$V_p$ (atm)	--	--	ND
$S$ (mg/L)	--	--	ND
$H$ (atm·m <sup>3</sup> /mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.05E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.69E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	1.17E+05
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.28E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.28E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.56E+02

TABLE A-3-170

## CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.10E+03
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.87E+03
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.46E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.55E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.55E-02
$Bv_{leafy\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$		B-2-8	ND
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$		B-3-8	ND



TABLE A-3-170

## CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.33E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.95E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.57E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.33E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.33E-03
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.53E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-02
$Oral CSF$ (mg/kg/day) <sup>-1</sup>		C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E-01
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>		C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-171

## CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	162.18
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	284.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.10E-04 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.50E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.19E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.06E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	7.16E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.57E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.68E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.68E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.26E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.73E+00

TABLE A-3-171

## CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.23E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.92E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.12E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.12E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.20E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.20E+00

TABLE A-3-171

## CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.63E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.15E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.39E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.63E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.06E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.19E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	1.80E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	5.10E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	1.80E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-172

## CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	78.96
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	490.1
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.03E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.20E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-172

## CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
<i>F<sub>v</sub></i> (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
<i>RCF</i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
<i>Br<sub>rootveg</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	2.20E-02
<i>Br<sub>ag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>ag</sub></i> value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. <i>Br<sub>ag</sub></i> value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average <i>Br<sub>ag</sub></i> value for aboveground produce was obtained as follows: (1) <i>Br<sub>ag</sub></i> values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) <i>Br<sub>ag</sub></i> values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.95E-02
<i>Br<sub>forage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>forage</sub></i> value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	1.60E-02
<i>Br<sub>grain</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>grain</sub></i> value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	2.00E-03
<i>B<sub>vag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-172

## CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
$B_{v_{forage}}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	5.86E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	2.27E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.88E-01
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	1.13E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	1.13E+00
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.29E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-03
Oral $CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E-02

TABLE A-3-172

## CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Inhalation <i>URF</i> ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup>	--	C-2-1	ND
Inhalation <i>CSF</i> ( $\text{mg}/\text{kg}/\text{day}$ ) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-173

## CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	107.87
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,233.6
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.38E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.71E-06
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND



TABLE A-3-173

## CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$F_v$ (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	1.00E-01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $B_v$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjöreen, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.38E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $B_v$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	4.00E-01
$Br_{grain}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjöreen, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjöreen, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	1.00E-01
$B_{v_{ag}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-173

## CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	Metals are assumed not to experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-02
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	3.0E-03
$Ba_{pork}$ (day/kg FW)	NC DEHNR (1997)	B-3-12	ND
$Ba_{egg}$ (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	2.04E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.80E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-174

## CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	334.40
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	541.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	2.20E-13 at 25°C (solid)
$S$ (mg/L)	Montgomery and Welkom (1991)	--	1.50E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.90E-13
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.38E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.58E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.51E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.53E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.53E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.40E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.81E+00

TABLE A-3-174

## CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg} \text{ (year)}^{-1}$	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.086
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis using a moisture content of 87 percent.	B-2-10	1.34E+01
$Br_{root \text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_{ds}$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.96E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.97E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.97E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.29E+07
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.29E+07

TABLE A-3-174

## CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.76E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.14E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	2.59E-06
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.76E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	1.69E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.72E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70kg.	C-2-3	1.1E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	---	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Note applicable  
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-175

## CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	104.14
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.5
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	8.21E-03 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.57E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.33E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.73E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.77E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.49E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.12E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.12E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.84E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.65E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.0



TABLE A-3-175

## CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.81E+01
$Br_{root\text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	5.28E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	7.85E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	7.85E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.21E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.21E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	6.74E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.13E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.58E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	6.74E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.68E-05

TABLE A-3-175

## CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	9.91E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	1.0E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-176

**CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN  
(1746-01-6)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	321.98
$T_m$ (K)	U.S. EPA (1994a)	--	578.1
$V_p$ (atm)	U.S. EPA (1994a)	--	4.45E-11 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	4.83E-04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.60E-05
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.27E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.81E-06
$K_{ow}$ (unitless)	U.S. EPA (1994a)	--	4.37E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.69E+04
$Kd_s$ (mL/g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.08E+05
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	4.29E-01

TABLE A-3-176

**CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN  
(1746-01-6)**

Parameter	Reference and Explanation	Equations	Value
<i>Fv</i> (unitless)	<i>Fv</i> value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of <i>Fv</i> was calculated by using <i>S</i> , <i>T<sub>m</sub></i> , and <i>Vp</i> values that are provided in this table. <i>Vp</i> value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	9.78E-01
<b>Biotransfer Factors for Plants</b>			
<i>RCF</i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	<i>RCF</i> value was calculated by using the correlation equation with <i>K<sub>ow</sub></i> that is cited in Briggs (1982). Recommended value was calculated by using the <i>K<sub>ow</sub></i> value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
<i>Br<sub>root veg</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>root veg</sub></i> value was calculated by dividing the <i>RCF</i> value with the <i>K<sub>d,s</sub></i> value provided in this table.	B-2-10	1.12E+00
<i>Br<sub>ag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>ag</sub></i> value was calculated by using the correlation equation with <i>K<sub>ow</sub></i> that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the <i>K<sub>ow</sub></i> value that is provided in this table.	B-2-9	5.62E-03
<i>Br<sub>forage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>forage</sub></i> value was calculated by using the correlation equation with <i>K<sub>ow</sub></i> that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the <i>K<sub>ow</sub></i> value that is provided in this table.	B-3-9	5.62E-03
<i>Bv<sub>ag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	<i>Bv<sub>ag</sub></i> value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	6.10E+04
<i>Bv<sub>forage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	<i>Bv<sub>forage</sub></i> value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	6.10E+04
<b>Biotransfer Factors for Animals</b>			
<i>Ba<sub>milk</sub></i> (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
<i>Ba<sub>beef</sub></i> (day/kg FW)	<i>Ba<sub>beef</sub></i> value was calculated by increasing <i>Ba<sub>milk</sub></i> values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
<i>Ba<sub>pork</sub></i> (day/kg FW)	<i>Ba<sub>pork</sub></i> value was calculated by increasing <i>Ba<sub>milk</sub></i> values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02

TABLE A-3-176

**CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN  
(1746-01-6)**

Parameter	Reference and Explanation	Equations	Value
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.42E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chickens}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.30E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	1.00
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)		C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-1-7	1.5E+05
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
Inhalation URF (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997c)	C-2-1	3.3E-08
Inhalation CSF (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997c)	C-2-2	1.5E+05

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-177

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	U.S. EPA (1994a)	--	305.98
$T_m$ (K)	U.S. EPA (1994a)	--	500.1
$V_p$ (atm)	U.S. EPA (1994a)	--	1.97E-11 at 25°C (solid)
$S$ (mg/L)	U.S. EPA (1994a)	--	4.19E-04
$H$ (atm·m <sup>3</sup> /mol)	U.S. EPA (1994a).	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.60E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.79E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.85E-06
$K_{ow}$ (unitless)	U.S. EPA (1992d)	--	3.39E+06
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.09E+06
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.09E+04
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.57E+05

TABLE A-3-177

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.36E+04
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	7.68E-01
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.48E+04
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.19E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.51E-03
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.51E-03
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.10E+04

TABLE A-3-177

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{forage}$ ( $\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}$ )	$Bv_{forage}$ value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.10E+04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	U.S. EPA (1995a)	B-3-11	3.00E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.63E-02
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by increasing $Ba_{milk}$ values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.97E-02
$Ba_{egg}$ (L/kg FW tissue)	$Ba_{egg}$ value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	3.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.63E-02
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
<b>Other Parameters</b>			
$TEF$ (unitless)	U.S. EPA (1994a)	--	0.10
<b>Health Benchmarks</b>			
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-8	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfD$ (mg/kg/day)	--	C-2-3	ND
$Inhalation\ URF$ ( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup>	--	C-2-1	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-2	ND

**TABLE A-3-177**

**CHEMICAL-SPECIFIC INPUTS FOR  
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)**

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-178

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	215.89
$T_m$ (K)	Montgomery and Welkom (1991)	--	411.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	7.1E-06 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.30E+00
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.18E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.11E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.75E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.36E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	5.89E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	2.36E+02



TABLE A-3-178

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.49E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.06E-02
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.06E-02
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.14E+00
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.14E+00
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.47E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.10E-03

TABLE A-3-178

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.33E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.66E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-03
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-179

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	167.85
$T_m$ (K)	Montgomery and Welkom (1991)	--	230.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b)	--	1.60E-02 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b)	--	1.10E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.44E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.15E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.27E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.59E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.59E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.20E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.37E+00
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0

TABLE A-3-179

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.09E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	1.94E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.17E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.17E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.45E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.45E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.39E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.07E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.30E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.39E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	8.46E-06

TABLE A-3-179

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	5.87E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.6E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	7.4E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	2.6E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-180

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	167.86
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	229.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.80E-03 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.07E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.72E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.16E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.26E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+04
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.90E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.90E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.93E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.16E+00



TABLE A-3-180

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.80E+02
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.11E+03
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.02E-02
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.02E-02
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.33E+01
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.33E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.50E-04

TABLE A-3-180

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.105E-03
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.34E-03
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.50E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	8.73E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.33E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	2.0E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	5.8E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	2.0E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-181

## CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	165.85
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	251.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	2.42E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	2.32E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.73E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.20E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	8.20E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.51E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.65E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.65E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.99E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.06E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.0

TABLE A-3-181

## CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.75E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.04E-03
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.31E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.31E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.66E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.66E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.79E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.82E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.07E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.79E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	6.96E-06

TABLE A-3-181

## CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	5.06E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997e)	C-1-7	5.2E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S.EPA (1997e)	C-2-1	5.8E-07
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S.EPA (1997e)	C-2-2	2.0E-03

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-182

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	U.S. EPA (1995b )	--	231.89																														
$T_m$ (K)	U.S. EPA (1995b)	--	343.0																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.60E-06 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+02																														
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.53E-05																														
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.55E-02																														
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	5.78E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.0E+04																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>6,190</td></tr><tr><td>2</td><td>6,188</td></tr><tr><td>3</td><td>6,166</td></tr><tr><td>4</td><td>5,956</td></tr><tr><td>5</td><td>4,456</td></tr><tr><td>6</td><td>1,323</td></tr><tr><td>7</td><td>249.2</td></tr><tr><td>8</td><td>115.3</td></tr><tr><td>9</td><td>101.6</td></tr><tr><td>10</td><td>100.2</td></tr><tr><td>11</td><td>100.0</td></tr><tr><td>12</td><td>100.0</td></tr><tr><td>13</td><td>100.0</td></tr><tr><td>14</td><td>100.0</td></tr></table>	pH	$K_{oc}$	1	6,190	2	6,188	3	6,166	4	5,956	5	4,456	6	1,323	7	249.2	8	115.3	9	101.6	10	100.2	11	100.0	12	100.0	13	100.0	14	100.0
pH	$K_{oc}$																																
1	6,190																																
2	6,188																																
3	6,166																																
4	5,956																																
5	4,456																																
6	1,323																																
7	249.2																																
8	115.3																																
9	101.6																																
10	100.2																																
11	100.0																																
12	100.0																																
13	100.0																																
14	100.0																																
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a $pH$ of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.49																														

TABLE A-3-182

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	18.69
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.97
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.83E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kds$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.94E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.27E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.27E-01

TABLE A-3-182

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{ag}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-9	1.39E+02
$Bv_{forage}$ $\left(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}}\right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.39E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.59E-04
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.02E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	6.08E-04
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.59E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.3 of Appendix A-3).	B-3-14	3.97E-04
$BCF_{fish}$ (L/kg, FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAF$ s were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCF$ s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCM$ s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.63E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-182

## CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
<b>Health Benchmarks</b>			
<i>RfD</i> (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
<i>Oral CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
<i>RfC</i> (mg/m <sup>3</sup> )	Calculated from <i>RfD</i> using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-01
<i>Inhalation URF</i> (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
<i>Inhalation CSF</i> (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-183

## CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	72.1
$T_m$ (K)	Montgomery and Welkom (1991)	--	164.6
$V_p$ (atm)	$V_p$ value cited in Budavari, O'Neil, Smith, and Heckleman (1989).	--	2.14E-01 at 25°C (liquid)
$S$ (mg/L)		--	ND
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.31E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.07E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	2.80E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	3.16E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.16E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.37E-01
Chemical/Physical Properties (Continued)			



TABLE A-3-183

## CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.26E-01
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	4.43E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.82E+00
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.16E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.14E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.14E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$		B-2-8	ND
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$		B-3-8	ND
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.22E-08

TABLE A-3-183

## CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	7.03E-08
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.51E-08
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.22E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.55E-08
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.29E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-184

## CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	204.38
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	576.6
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.48E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.34E-06
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-184

## CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
$F_v$ (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
Biotransfer Factors for Plants			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	B-2-10	ND
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{rootveg}$ .	B-2-10	4.00E-04
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value for fruits was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{ag}$ (fruits). $Br_{ag}$ value for vegetables was calculated using data obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative (reproductive) growth and $B_v$ values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoeren, and Shor [1984])—were used for $Br_{ag}$ (vegetables). The weighted average $Br_{ag}$ value for aboveground produce was obtained as follows: (1) $Br_{ag}$ values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) $Br_{ag}$ values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	8.58E-04
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $B_v$ values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{forage}$ .	B-3-8	4.00E-03
$Br_{grain}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{grain}$ value was obtained from Baes, Sharp, Sjoeren, and Shor (1984). $Br$ values for nonvegetative growth as recommended by Baes, Sharp, Sjoeren, and Shor (1984) were used for $Br_{grain}$ .	B-3-8	4.00E-04
$B_{v_{ag}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
$B_{v_{forage}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-184

## CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-03
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	4.0E-02
$Ba_{pork}$ (day/kg FW)	--	B-3-12	ND
$Ba_{eggs}$ (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.40E+03
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-05
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.8E-04
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-185

## CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	92.13
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.71E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	5.58E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.13E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.72E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.23E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	4.65E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.40E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.40E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.60E+00
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.15E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.0

TABLE A-3-185

## CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.26E+01
$Br_{root\text{ veg}}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\text{ veg}}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.33E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.11E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.11E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.33E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.33E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.69E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.17E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.41E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.69E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.22E-06

TABLE A-3-185

## CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.27E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	4.0E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-186

## CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	107.15
$T_m$ (K)	Montgomery and Welkom (1991)	--	258.4
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	3.94E-04 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.74E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.14E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.12E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.19E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.57E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.57E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.18E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.28E-01

TABLE A-3-186

## CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.81E+00
$Br_{root \text{ veg}}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	5.61E+01
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.51E+00
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.51E+00
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	6.16E-01
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	6.16E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.74E-07

TABLE A-3-186

## CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	5.50E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	6.65E-07
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.74E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	4.34E-07
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.14E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	NA
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	2.4E-01
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	NA
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	6.9E-02
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	2.4E-01

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-187

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	325.7
$V_p$ (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	3.20E-04 at 25°C (solid)
$S$ (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	2.05E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.84E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.02E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.15E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.11E+04
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.02E+04
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.02E+02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.52E+03
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	8.10E+02

TABLE A-3-187

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $T_m$ and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	3.09E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_{ds}$ value provided in this table.	B-2-10	1.53E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.78E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.78E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	4.01E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	4.01E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	8.82E-05

TABLE A-3-187

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.79E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	3.38E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	8.82E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.20E-04
$BCF_{fish}$ (L/kg FW tissue)	--	B-4-26	NA
$BAF_{fish}$ (L/kg FW)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with an estimated $BCF$ . $BCFs$ were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	8.76E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-188

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	290.1
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	4.42E-04 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	3.07E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.61E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.00E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.23E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	9.73E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.66E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.66E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.24E+02
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.64E+01
<b>Chemical/Physical Properties (Continued)</b>			
$ksg$ (year) <sup>-1</sup>	$ksg$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
$Fv$ (unitless)	$Fv$ value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.0

TABLE A-3-188

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.80E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.69E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.92E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.92E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.78E-01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.78E-01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	7.73E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	2.45E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.96E-04
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	7.73E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.93E-04



TABLE A-3-188

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	6.33E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	2.0E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable  
 ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-189

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.7
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.63E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.17E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.86E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.66E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.56E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.64E+02
$K_{oc}$ (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	--	1.35E+05
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.35E+03
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.01E+04
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.40E+03
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.26E-01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided	B-1-1; B-2-1; B-2-7; B-2-8;	1.00

TABLE A-3-189

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	2.33E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.73E-02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.54E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.54E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.14E-03
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.14-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.10E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.63E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.03E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.10E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.24E-06

TABLE A-3-189

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.08E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.50E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	NA
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.23E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	NA
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	NA

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-190

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	238.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.31E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.51E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E+02
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.50E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.50E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.63E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.00E+00

TABLE A-3-190

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.93E-01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.59E+01
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.38E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.38E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	9.53E-03
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	9.53E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	9.93E-07

TABLE A-3-190

## CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.14E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	3.80E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	9.93E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	2.48E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.31E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	5.70E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.4E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997b)	C-2-1	1.6E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	5.7E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-191

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	131.40
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	188.3
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.48E-02 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.18E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.06E-02
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.65E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.94E-06
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.71E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	9.40E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.40E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.05E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.76E+00

TABLE A-3-191

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.703
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.37E+01
$Br_{root \text{ veg}}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.52E+00
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.52E+00
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.07E-03
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.07E-03
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.15E-06

TABLE A-3-191

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.81E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	8.24E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	5.37E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.16E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997a)	C-1-8	6.0E-03
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	1.1E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.1E-02
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1995b)	C-2-1	1.7E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral\ CSF$ assuming route-to-route extrapolation.	C-2-2	1.1E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-192

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	137.38
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	162.1
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.10E+00 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.10E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.37E-01
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.27E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
$K_{ow}$ (unitless)	$K_{ow}$ value cited in U.S. EPA (1995b).	--	3.40E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.34E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.34E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.00E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	5.34E+00

TABLE A-3-192

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/mL \text{ soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.70E+01
$Br_{root \text{ veg}}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{root \text{ veg}}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.02E+00
$Br_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.33E+00
$Br_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.33E+00
$Bv_{ag}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.02E-04
$Bv_{forage}$ $(\frac{\mu g/g \text{ DW plant}}{\mu g/g \text{ air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.02E-04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.70E-06

TABLE A-3-192

## CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	8.54E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.2 of Appendix A-3).	B-3-12	1.03E-05
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.70E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A3.4.3 of Appendix A-3).	B-3-14	6.74E-06
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.94E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997c)	C-2-3	7.0E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-193

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	197.46																														
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	340.1																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.15E-05 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02																														
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.64E-06																														
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.91E-02																														
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.03E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.41E+03																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>2,380</td></tr><tr><td>2</td><td>2,380</td></tr><tr><td>3</td><td>2,380</td></tr><tr><td>4</td><td>2,377</td></tr><tr><td>5</td><td>2,353</td></tr><tr><td>6</td><td>2,139</td></tr><tr><td>7</td><td>1,127</td></tr><tr><td>8</td><td>223.7</td></tr><tr><td>9</td><td>56.14</td></tr><tr><td>10</td><td>37.94</td></tr><tr><td>11</td><td>36.10</td></tr><tr><td>12</td><td>35.92</td></tr><tr><td>13</td><td>35.90</td></tr><tr><td>14</td><td>35.90</td></tr></table>	pH	$K_{oc}$	1	2,380	2	2,380	3	2,380	4	2,377	5	2,353	6	2,139	7	1,127	8	223.7	9	56.14	10	37.94	11	36.10	12	35.92	13	35.90	14	35.90
pH	$K_{oc}$																																
1	2,380																																
2	2,380																																
3	2,380																																
4	2,377																																
5	2,353																																
6	2,139																																
7	1,127																																
8	223.7																																
9	56.14																																
10	37.94																																
11	36.10																																
12	35.92																																
13	35.90																																
14	35.90																																
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.13E+01																														
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	8.45E+01																														



TABLE A-3-193

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	4.51E+01
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.367
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.28E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	2.02E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.24E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.24E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.31E+02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.31E+02

TABLE A-3-193

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	5.89E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.86E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	2.25E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	5.89E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.47E-04
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	5.14E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	3.5E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable  
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-194

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value																														
Chemical/Physical Properties																																	
$MW$ (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	197.46																														
$T_m$ (K)	Budavari, O’Neil, Smith, and Heckelman (1989)	--	342.1																														
$Vp$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.55E-05 at 25°C (solid)																														
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02																														
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.06E-06																														
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02																														
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.08E-06																														
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.15E+03																														
$K_{oc}$ (mL/g)	For all ionizing organics, $K_{oc}$ values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	<table><tr><th>pH</th><th><math>K_{oc}</math></th></tr><tr><td>1</td><td>1,070</td></tr><tr><td>2</td><td>1,070</td></tr><tr><td>3</td><td>1,069</td></tr><tr><td>4</td><td>1,063</td></tr><tr><td>5</td><td>1,006</td></tr><tr><td>6</td><td>670.8</td></tr><tr><td>7</td><td>226.2</td></tr><tr><td>8</td><td>120.4</td></tr><tr><td>9</td><td>108.4</td></tr><tr><td>10</td><td>107.1</td></tr><tr><td>11</td><td>107.0</td></tr><tr><td>12</td><td>107.0</td></tr><tr><td>13</td><td>107.0</td></tr><tr><td>14</td><td>107.0</td></tr></table>	pH	$K_{oc}$	1	1,070	2	1,070	3	1,069	4	1,063	5	1,006	6	670.8	7	226.2	8	120.4	9	108.4	10	107.1	11	107.0	12	107.0	13	107.0	14	107.0
pH	$K_{oc}$																																
1	1,070																																
2	1,070																																
3	1,069																																
4	1,063																																
5	1,006																																
6	670.8																																
7	226.2																																
8	120.4																																
9	108.4																																
10	107.1																																
11	107.0																																
12	107.0																																
13	107.0																																
14	107.0																																
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.26E+00																														

TABLE A-3-194

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	1.70E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.05E+00
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+00
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.74E+02
$Br_{root\ veg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	7.69E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	2.77E-01
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	2.77E-01

TABLE A-3-194

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants (Continued)</b>			
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.23E+02
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.23E+02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	4.09E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.29E-04
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.57E-04
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	4.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	1.02E-04
$BCF_{fish}$ (L/kg, FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.90E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	--	C-1-8	--
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1995b)	C-1-7	1.1E-02
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	--
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997)	C-2-1	3.1E-06
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	--

## TABLE A-3-194

### CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

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TABLE A-3-195

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Montgomery and Welkom (1991)	--	147.43
$T_m$ (K)	Montgomery and Welkom (1991)	--	258.4
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	4.90E-03 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	1.90E+03
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.80E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.99E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.24E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+02
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	8.05E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.10E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.04E+00
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	3.22E+00



TABLE A-3-195

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$k_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.89E+01
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.34E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.94E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.94E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	3.66E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.66E-02
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.41E-06
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	4.47E-06

TABLE A-3-195

## CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	5.41E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.41E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.53E-06
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	3.02E+01
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-03
$Oral CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	7.0E+00
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	2.1E-02
$Inhalation URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	2.0E-03
$Inhalation CSF$ (mg/kg/day) <sup>-1</sup>	Value based on $Oral CSF$ assuming route-to-route extrapolation.	C-2-2	7.0E+00

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-196

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.19
$T_m$ (K)	Montgomery and Welkom (1991)	--	287.9
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.30E-03 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	2.00E+01
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.81E-03
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.48E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.86E-06
$K_{ow}$ (unitless)	$K_{ow}$ value cited in Howard (1989-1993).	--	2.63E+03
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.67E+03
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.67E+01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.25E+02
<b>Chemical/Physical Properties (Continued)</b>			

TABLE A-3-196

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	6.69E+01
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	3.16E+01
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+02
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	6.35E+00
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.09E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.09E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.14E-02
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	3.14E-02

TABLE A-3-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	2.09E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	6.61E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	8.00E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	2.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	5.22E-05
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.34E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997a)	C-1-8	5.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>		C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>		C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>		C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-197

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	213.11
$T_m$ (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	395.6
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1995b).	--	1.30E-07 at 25°C (solid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1995b).	--	3.20E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.66E-08
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.84E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	6.08E-06
$K_{ow}$ (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.51E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.18E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.18E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.84E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.72E-01



TABLE A-3-197

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $F_v$ was calculated by using $S$ , $T_m$ , and $V_p$ values that are provided in this table. $V_p$ value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.19E+00
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	6.95E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.05E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.05E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.17E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature ( $T$ ) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.17E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.20E-07



TABLE A-3-197

## CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.80E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.60E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.20E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.00E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	4.64E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-198

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	227.13
$T_m$ (K)	Montgomery and Welkom (1991)	--	353.2
$V_p$ (atm)	--	--	ND
$S$ (mg/L)	--	--	ND
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.85E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	3.98E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	2.51E+01
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.51E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.88E+00
<b>Chemical/Physical Properties (Continued)</b>			

TABLE A-3-198

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.00E+00
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
$F_v$ (unitless)	$F_v$ value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}})$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.03E+01
$Br_{rootveg}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	4.10E+01
$Br_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	4.60E+00
$Br_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}})$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	4.60E+00
$Bv_{ag}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	--	B-2-8	ND
$Bv_{forage}$ $(\frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}})$	--	B-3-8	ND

TABLE A-3-198

## CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.16E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.00E-06
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.21E-06
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.16E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	7.89E-07
$BCF_{fish}$ (L/kg FW tissue)	$BCF$ s were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	9.68E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-1-7	3.0E-02
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.8E-03
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	Calculated from $Oral\ CSF$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-1	8.6E-06
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997b)	C-2-2	3.0E-02

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-199

## CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	86.09
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	180.1
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.43E-01 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.24E+04
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.50E-04
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.94E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.00E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.00E+00
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	4.97E+00
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.97E-02
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.73E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.99E-01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0

TABLE A-3-199

## CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.11E+00
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	1.43E+02
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	1.53E+01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	1.53E+01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	5.65E-04
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	5.65E-04
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	3.97E-08
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	1.26E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	1.52E-07
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	3.97E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	9.92E-08

TABLE A-3-199

## CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	2.00E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E+00
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	U.S. EPA (1997b)	C-2-3	2.0E-01
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA= Not applicable

ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-200

## CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	62.50
$T_m$ (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	119.3
$V_p$ (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.68E+00 at 25°C (liquid)
$S$ (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.30E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.15E-01
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.58E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.19E-05
$K_{ow}$ (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.40E+01
$K_{oc}$ (mL/g)	$K_{oc}$ value was calculated by using the correlation equation with $K_{ow}$ for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). $K_{oc}$ value was calculated by using the recommended $K_{ow}$ value that is provided in this table.	--	1.11E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.11E-01
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.32E-01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	4.44E-01
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00

TABLE A-3-200

## CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.08E+00
$Br_{root\ veg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{root\ veg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	7.29E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	8.42E+00
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	8.42E+00
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci and others (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	2.95E-06
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	2.95E-06
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.11E-07
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.52E-07
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-12	4.26E-07

TABLE A-3-200

## CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
$Ba_{eggs}$ (day/kg FW)	$Ba_{eggs}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.11E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value (see section A4.3.2 of Appendix A-3).	B-3-14	2.78E-07
$BCF_{fish}$ (L/kg, FW tissue)	$BAFs$ were used for compounds with a log $K_{ow}$ value above 4.0, as cited in U.S. EPA (1995b). $BAF$ values were predicted values calculated by multiplying a food chain multiplier ( $FCM$ ) with a geometric mean of various laboratory measured $BCFs$ obtained from various experimental studies cited in U.S. EPA (1998). $FCMs$ were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-26	4.37E+00
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
$RfD$ (mg/kg/day)	--	C-1-8	ND
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-1-7	1.9E+00
$RfC$ (mg/m <sup>3</sup> )	--	C-2-3	ND
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	U.S. EPA (1997c)	C-2-1	8.4E-05
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	U.S. EPA (1997c)	C-2-2	3.0E-01

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
$T_m$ (K)	Montgomery and Welkom (1991)	--	225.7
$V_p$ (atm)	$V_p$ value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	1.60E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $V_p$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.26E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.49E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	1.59E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.96E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.96E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.47E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	7.84E+00
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
$F_v$ (unitless)	$F_v$ value was calculated by using the equation cited in Junge (1977). Recommended value of $F_v$ was calculated by using the $V_p$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8;	1.000

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.41E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $Kd_s$ value provided in this table.	B-2-10	3.78E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.47E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.47E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.55E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.55E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.26E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.99E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.83E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.26E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	3.15E-05

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.60E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.



TABLE A-3-202

## CHEMICAL-SPECIFIC INPUTS FOR O-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
$T_m$ (K)	Montgomery and Welkom (1991)	--	248.1
$Vp$ (atm)	$Vp$ value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	2.20E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.73E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.44E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	1.35E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.41E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.41E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.81E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	9.64E+00
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
$Fv$ (unitless)	$Fv$ value was calculated by using the equation cited in Junge (1977). Recommended value of $Fv$ was calculated by using the $Vp$ value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8;	1.000



TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.61E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.74E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	6.01E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	6.01E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.79E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.79E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.07E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.39E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.10E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.07E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.68E-05

TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.41E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-203

## CHEMICAL-SPECIFIC INPUTS FOR P-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
$T_m$ (K)	Montgomery and Welkom (1991)	--	286.1
$Vp$ (atm)	$Vp$ value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
$S$ (mg/L)	$S$ value cited in U.S. EPA (1992a).	--	2.15E+02
$H$ (atm·m <sup>3</sup> /mol)	$H$ value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the $MW$ , $S$ , and $Vp$ values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.89E-06
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.61E+02
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.50E-06
$K_{ow}$ (unitless)	Recommended $K_{ow}$ value cited in Karickhoff and Long (1995).	--	1.48E+03
$K_{oc}$ (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.11E+02
$Kd_s$ (cm <sup>3</sup> /g)	$Kd_s$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate $Kd_s$ , because the value varies, depending on the fraction of organic carbon in soil. Recommended $Kd_s$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.11E+00
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate $Kd_{sw}$ , because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended $Kd_{sw}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.33E+01
$Kd_{bs}$ (cm <sup>3</sup> /g)	$Kd_{bs}$ value was calculated by using the correlation equation with $K_{oc}$ that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate $Kd_{bs}$ , because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended $Kd_{bs}$ value was calculated by using the $K_{oc}$ value that is provided in this table.	B-4-16; B-4-25	1.24E+01
<b>Chemical/Physical Properties (Continued)</b>			
$k_{sg}$ (year) <sup>-1</sup>	$K_{sg}$ value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
$Fv$ (unitless)	$Fv$ value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of $Fv$ was calculated by using $T_m$ and $Vp$ values that	B-1-1; B-2-1; B-2-7; B-2-8;	1.00

TABLE A-3-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Plants</b>			
$RCF$ $\left( \frac{\mu\text{g/g WW plant}}{\mu\text{g/mL soil water}} \right)$	$RCF$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Briggs (1982). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-10	7.05E+01
$Br_{rootveg}$ $\left( \frac{\mu\text{g/g WW plant}}{\mu\text{g/g soil}} \right)$	$Br_{rootveg}$ value was calculated by dividing the $RCF$ value with the $K_d$ value provided in this table.	B-2-10	2.27E+01
$Br_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-2-9	5.70E-01
$Br_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	$Br_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-9	5.70E-01
$Bv_{ag}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{ag}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-2-8	1.93E+01
$Bv_{forage}$ $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	$Bv_{forage}$ value was calculated by using the correlation equation with $K_{ow}$ and $H$ that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the $H$ and $K_{ow}$ values that are provided in this table.	B-3-8	1.93E+01
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-11	1.18E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in Travis and Arms (1988). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-10	3.72E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the $Ba_{beef}$ value.	B-3-12	4.50E-05
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ value was calculated by using the correlation equation with $K_{ow}$ that is cited in California EPA (1993). Recommended value was calculated by using the $K_{ow}$ value that is provided in this table.	B-3-13	1.18E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the $Ba_{beef}$ value.	B-3-14	2.93E-05

TABLE A-3-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
$BCF_{fish}$ (L/kg FW tissue)	$BCFs$ were used for compounds with a log $K_{ow}$ value below 4.0, as cited in U.S. EPA (1995b). $BCF_{fish}$ value calculated using the correlation equation with $K_{ow}$ obtained from Veith, Macek, Petrocelli, and Carroll (1980)—See Appendix A-3.	B-4-26	1.51E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	7.0E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note:

NA = Not applicable

ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-204

## CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties</b>			
$MW$ (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	65.38
$T_m$ (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	692.6
$V_p$ (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
$S$ (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	--	0.0
$H$ (atm·m <sup>3</sup> /mol)	$H$ value is assumed to be zero, because the $V_p$ and $S$ values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
$D_a$ (cm <sup>2</sup> /s)	$D_a$ value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.17E-01
$D_w$ (cm <sup>2</sup> /s)	$D_w$ value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.36E-05
$K_{ow}$ (unitless)	--	--	NA
$K_{oc}$ (mL/g)	--	--	NA
$Kd_s$ (mL/g)	$Kd_s$ value was obtained from U.S. EPA (1996), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.2E+01 at pH=6.8
$Kd_{sw}$ (L/Kg)	$Kd_{sw}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	6.2E+01 at pH=6.8
$Kd_{bs}$ (mL/g)	$Kd_{bs}$ value is assumed to be same as the $Kd_s$ value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	6.2E+01 at pH=6.8
$k_{sg}$ (year) <sup>-1</sup>	--	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	ND

TABLE A-3-204

## CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
<b>Chemical/Physical Properties (Continued)</b>			
<i>F<sub>v</sub></i> (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
<b>Biotransfer Factors for Plants</b>			
<i>RCF</i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/mL soil water}} \right)$	--	--	ND
<i>Br<sub>rootveg</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	4.40E-02
<i>Br<sub>ag</sub></i> (fruit) $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for garden fruits.	B-2-9	4.60E-02
<i>Br<sub>ag</sub></i> (veg) $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b).	B-3-9	9.70E-02
<i>Br<sub>forage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-9	2.50E-01
<i>Br<sub>grain</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g soil}} \right)$	<i>Br<sub>rootveg</sub></i> value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10 <sup>9</sup> g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-9	5.40E-02
<i>B<sub>vag</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
<i>B<sub>vforage</sub></i> $\left( \frac{\mu\text{g/g DW plant}}{\mu\text{g/g air}} \right)$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA



TABLE A-3-204

## CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
<b>Biotransfer Factors for Animals</b>			
$Ba_{milk}$ (day/kg FW)	$Ba_{milk}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	3.25E-05
$Ba_{beef}$ (day/kg FW)	$Ba_{beef}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	9.00E-05
$Ba_{pork}$ (day/kg FW)	$Ba_{pork}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.28E-04
$Ba_{egg}$ (day/kg FW)	$Ba_{egg}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	8.75E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	8.75E-03
$BCF_{fish}$ (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4.).	B-4-26	6.54E+02
$BAF_{fish}$ (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
<b>Health Benchmarks</b>			
$RfD$ (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
$Oral\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-1-7	ND
$RfC$ (mg/m <sup>3</sup> )	Calculated from $RfD$ using an inhalation rate of 20 m <sup>3</sup> /day and a human body weight of 70 kg.	C-2-3	1.1E+00
$Inhalation\ URF$ (μg/m <sup>3</sup> ) <sup>-1</sup>	--	C-2-1	ND
$Inhalation\ CSF$ (mg/kg/day) <sup>-1</sup>	--	C-2-2	ND

Note: NA = Not applicable; ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.